

Giant magnetic enhancement in Fe/Pd films and its influence on the magnetic interlayer coupling

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The magnetic properties of thin Pd fcc(001) films with embedded monolayers of Fe are investigated by means of first principles density functional theory. The induced spin polarization in Pd is calculated and analyzed in terms of quantum interference within the Fe/Pd/Fe bilayer system. An investigation of the magnetic enhancement effects on the spin polarization is carried out and its consequences for the magnetic interlayer coupling are discussed. In contrast to *e.g.* the Co/Cu fcc(001) system we find a large effect on the magnetic interlayer coupling due to magnetic enhancement in the spacer material. In the case of a single embedded Fe monolayer we find an induced Pd magnetization decaying with distance n from the magnetic layer as $n^{-\alpha}$ with $\alpha \approx 2.4$. For the bilayer system we find a giant magnetic enhancement (GME) that oscillates strongly due to interference effects. This results in a strongly modified magnetic interlayer coupling, both in phase and magnitude, which may not be described in the pure Ruderman-Kittel-Kasuya-Yoshida (RKKY) picture. No anti-ferromagnetic coupling was found and by comparison with magnetically constrained calculations we show that the overall ferromagnetic coupling can be understood from the strong polarization of the Pd spacer.

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INTRODUCTION

In order to understand itinerant magnetism, paramagnetic materials with a high spin susceptibility are of special interest. These materials are on the border of being ferromagnetic and small perturbations may therefore lead to a spontaneous spin polarization. A reduction of the dimension may, for example, induce a magnetic moment in thin Pd films placed on Ag fcc(001) as a result of the finite size effects in the Pd film [1]. Another example is the large polarization cloud around Fe impurities in Pd. The cloud has a radius of about 10 Å and a total magnetic moment of 12 μ_B [2]. The moment of the Fe impurity itself is on the order of 3 μ_B which means that about 9 μ_B is coming from the induced moments in Pd. The effect can theoretically be understood in terms of enhancement of the paramagnetic Pauli spin susceptibility that strongly modifies the magnetic properties of the unperturbed paramagnetic ground state. In this paper we investigate the magnetization of Pd when the Fe impurity is substituted by a two-dimensional layer. We also analyze the magnetic interaction, i.e. the magnetic interlayer coupling (MIC) between two separate monolayers of Fe in a Pd host. This could lead to large moments of the embedded Pd host. In that case the electronic structure of Pd may be strongly modified and the Ruderman, Kittel, Kasuya, Yoshida (RKKY) or quantum-well (QW) like theories describing the magnetic interlayer coupling that are based on the properties of the unperturbed paramagnetic spacer bulk material may break down, c.f. the Fe/Cr/Fe system [3].

The MIC has attracted a lot of interest since its discovery by Grünberg *et al.* in 1986 [4]. It is a long range interaction between magnetic layers through paramagnetic spacer material and combined with the giant magnetoresistance effect [5] it is one of the main mechanisms in magnetic sensor and memory devices. The MIC is theoretically well understood [6, 7, 8, 9] for the case of a paramagnetic, insulating or disordered alloy spacer and it has been shown to be well described by the RKKY [10, 11, 12] coupling originally explaining the interaction between local magnetic impurities in a paramagnetic host. A related way of describing the MIC is the QW picture [13, 14, 15, 16], where the coupling is viewed in terms of confined states in the spacer that have different energies depending on spacer thickness and orientation between the magnetic layers.

In the last ten years the Fe/Pd multilayers has drawn a lot of attention, mostly because the first measurements indicated a weak anti-ferromagnetic (AFM) coupling for spacer thicknesses around 12 monolayers (ML) in a Fe_{5.7}/Pd_x/Fe_{9.6} (100) system (Celinski *et al.* [17]) that looked very promising for applications. Later Childress *et al.* [18] investigated the same system and found no trace of an AFM coupling in the thickness range from ~ 5 to 25 ML. They also noted that a weak in-plane uniaxial anisotropy that changes with spacer thickness may be mistaken for an AFM coupling. However, in the latest experiment on the MIC, Lucic *et al.* found a strong AFM coupling for a Pd thickness of 6 ML [19]. Lucic also showed that the interface morphology plays an important role and that the AFM peaks are only present in samples

with very smooth interfaces (~ 1000 nm size terraces). The switching from ferromagnetic (FM) to AFM coupling also agrees with the calculated results by Stoeffer *et al.* for one of their considered structures of the Pd spacer, the constant atomic volume structure (CAV). In this structure the Pd maintains its bulk volume but adapts the interplanar distance in order to fit the Fe bcc(100) interface [20]. The results by Stoeffer *et al.* are for spacer thicknesses up to 6 ML so the width of this AFM region cannot be determined. The results up to now on the MIC, both experimental and theoretical have been on multilayers with thick bcc (100) Fe layers sandwiched with fcc (100) Pd. Recently Cros *et al.* found a high spin Fe phase in Fe/Pd(100) when the Fe layers are very thin (1 to 3 ML). They also found that the Fe layers adapt to the Pd fcc structure with almost the same lattice constant [21].

This paper is outlined as follows. Firstly, we present some calculational details, where we describe the linear muffin-tin orbitals (LMTO) Green's function technique used in the density functional calculations, then we describe how effects due to multiple scattering, *i.e.* interface interference terms, can be extracted and analyzed separately, and how magnetic enhancement effects can be estimated by a comparison with magnetically quenched calculations. Thereafter we show the result of the magnetization induced in Pd from a planar interface perturbation that is a single monolayer of Fe fcc (001) embedded in the Pd fcc host. In the next section we calculate the induced magnetization of the bilayer system, with two separate Fe monolayers embedded in the Pd host, and we estimate the effect due to interface interference. Subsequent to that, the magnetization results are discussed in terms of quantum well states. At the end we present the calculated MIC and by a comparison with magnetically constrained calculations and the MIC of the Co/Cu system we discuss the possibility to apply RKKY theory for describing the magnetic interlayer coupling in magnetically enhanced multilayers.

CALCULATIONAL DETAILS

Total energy calculations

The *ab initio* density functional calculations were performed within the local spin density approximation applying an interface Green's function technique developed by Skriver and Rosengaard [22]. The method is based on the LMTO method [23, 24] within the tight-binding [25], frozen core, and atomic-sphere approximations. The local spin density approximation as parameterized by Vosko, Wilk, and Nusair [26] was used. An advantage of the Green's function technique is that it ensures a correct description of the loss of translational symmetry perpendicular to the interface, without the use of an artificial

slab or supercell geometry. The studied bilayers consist of two layers of Fe with a thickness of 1 ML embedded in bulk Pd. The Fe layers are separated by N layers of Pd, where $1 \leq N \leq 16$. All calculations were performed in the Pd bulk fcc lattice with a lattice constant $a=3.89$ Å, neglecting structure relaxations. The direction of growth was (100). This particular choice of structure is justified by the results by Cros *et al.* [21].

The MIC was calculated as the difference in total energy between the situation of AFM aligned Fe layers and the system with FM aligned Fe layers

$$J_{MIC}(N) = E_{AFM}^{tot}(N) - E_{FM}^{tot}(N). \quad (1)$$

Furthermore, we found that 528 special k-points were needed in the irreducible part of the 2-dimensional Brillouin zone to obtain k-point convergence of the MIC.

Multiple scattering contribution to the magnetic moment

To analyze the multiple scattering contribution to the magnetic moment in the spacer the method by Niklasson *et al.* described in detail in ref. [14] was used. The main idea is that the perturbed Green's function of the embedded Pd film G^σ can be expressed in terms of the corresponding unperturbed paramagnetic bulk Green's function G_0 as

$$G^\sigma = G_0 + \Delta G_L^\sigma + \Delta G_R^\sigma + \Delta G_{QW}^\sigma. \quad (2)$$

Here ΔG_L^σ and ΔG_R^σ are the independent planar perturbations arising from the two non-interacting Fe monolayers, and ΔG_{QW}^σ is the term due to interference in the QW like structure formed by the Fe/Pd/Fe system. By subtracting a superposition of the independent magnetic interface perturbations, calculated from a single Fe ML embedded in the Pd host, from the magnetization profile of the fully interacting Fe/Pd/Fe bilayer system the contribution to the magnetic moment from the interference term can be estimated. In this way the effects of quantum interference on the polarization of the spacer due to the occurrence of confined, so called QW states, can be separated and analyzed.

Magnetic enhancement

When a material is exposed to a magnetic field its magnetization is determined by the magnetic susceptibility. However, the magnetization of the material induces an internal magnetic field that influences the neighbouring atoms and the resulting magnetization is determined by the response to the sum of the applied field and the induced field inside the material. This "self-consistency effect" is referred to as exchange enhancement and is large

in elements with a high susceptibility such as Palladium. The enhanced susceptibility can be estimated from the un-enhanced Pauli spin susceptibility, χ_0 , by

$$\chi = \frac{\chi_0}{1 - I\chi_0} \quad (3)$$

where I is the Stoner exchange parameter that specifies the intra-atomic magnetic coupling in the material. The exchange enhancement, that may lead to a complete change of the electronic structure, is hard to estimate and is generally not included in, for example, the RKKY theory describing the magnetic interlayer coupling in magnetic multilayers. It is thus of great interest to try to understand the magnitude of this effect.

Methods of obtaining the MIC that use the force theorem or frozen potentials for the spacer atoms are based on the RKKY description of the MIC and although very successful for calculating asymptotic behaviour for many multilayer systems, they do not take the enhanced susceptibility into account. For technical reasons, we cannot employ this type of approximations directly in our computer program and in order to mimic such an approach we have imposed a constraint $\chi = \chi_0$, *i.e.* $I = 0$, that we from now refer to as the quenched case.

This limit can be achieved by imposing the condition that the exchange correlation potential for some, or all Pd atoms in the system only contains the paramagnetic part. It is important to notice that since the magnetic moments are determined by the Green's function for the whole sample there will still be nonzero magnetic moments on the quenched Pd atoms. The Pd magnetization is quenched in order to critically test whether a perturbation around a paramagnetic ground state is valid, as in a RKKY model.

RESULTS

Interface Induced Magnetization

In Table I we show the calculated magnetic profile of one embedded Fe layer in Pd in the case of enhanced and quenched Pd atoms. The profile corresponds to a calculation of the magnetic moments from the ΔG_L^{σ} terms in eq.(2).

In the enhanced situation one can see that there is a weak oscillation of the Pd moments around a positive value and a decay with the distance n monolayers from the magnetic layer. The findings are in agreement with results for Fe impurities in Pd, both experimental [2] and theoretical [27]. By a least square fit of the calculated enhanced profile to the approximate decaying sinusoidal description $\sim n^{-\alpha}(C \sin(\beta n + \Phi) + \xi)$ we find that $\alpha \approx 2.4$, $C \approx 0.63$, $\beta \approx 1.11$, $\Phi \approx 3.5$ and $\xi \approx 0.96$. In the quenched situation, the positive bias has disappeared

Layer	Enhanced	Quenched	Layer	Enhanced	Quenched
<i>Fe</i>	3.0378	3.0512	<i>Pd</i> ₁₀	0.0026	-0.0005
<i>Pd</i> ₁	0.3330	0.2251	<i>Pd</i> ₁₁	0.0005	0.0012
<i>Pd</i> ₂	0.1396	0.0412	<i>Pd</i> ₁₂	0.0006	0.0015
<i>Pd</i> ₃	0.0978	0.0048	<i>Pd</i> ₁₃	0.0021	0.0005
<i>Pd</i> ₄	0.0561	-0.0029	<i>Pd</i> ₁₄	0.0029	-0.0007
<i>Pd</i> ₅	0.0236	-0.0002	<i>Pd</i> ₁₅	0.0018	-0.0008
<i>Pd</i> ₆	0.0079	0.0026	<i>Pd</i> ₁₆	0.0004	0.0001
<i>Pd</i> ₇	0.0053	0.0004	<i>Pd</i> ₁₇	0.0000	0.0008
<i>Pd</i> ₈	0.0067	-0.0018	<i>Pd</i> ₁₈	0.0005	0.0006
<i>Pd</i> ₉	0.0053	-0.0021	<i>Pd</i> ₁₉	0.0009	-0.0001

TABLE I: The magnetic profile of the $\text{Pd}_{\infty}/\text{Fe}_1/\text{Pd}_{\infty}$ system as calculated with unconstrained susceptibility (Enhanced) and constrained to the un-enhanced Pauli susceptibility on the Pd atoms (Quenched). The unit is μ_B/atom .

and the magnetic profile oscillates around the zero level but the interface Pd atom still maintains most of its polarization. Worth pointing out here is that the decay is here obtained from a fit to all moments including the interface Pd atom and does not necessarily describe the exact asymptotic result.

Moving on to the case of two embedded Fe layers we see in Fig.(1) the total magnetic moment of the spacer together with the superposition of magnetic profiles from a single Fe monolayer in Pd. The figure shows the results from calculations where all Pd atoms are quenched, when the interface Pd atoms are left enhanced and when all Pd atoms are enhanced. In all cases the superimposed curves reach a finite, positive value, the completely quenched curve about $0.5\mu_B$, the interface enhanced curve $0.75\mu_B$ and the enhanced curve about $1.2\mu_B$. The constant value is reached faster in the completely quenched case, already at 2 ML spacer thickness compared to the enhanced case where the constant value is reached at about 5 ML. This effect is natural since the polarization of Pd in the case of one embedded Fe ML is stronger and more long range in the enhanced case compared to the quenched case (see Table I). The shift between the enhanced and completely quenched superimposed curves is about $0.7\mu_B$ which must then be attributed to enhancement in Pd in the absence of multiple interface scattering effects. This is a giant magnetic enhancement (GME) effect which is completely absent in the case of the corresponding Co/Cu system where the enhanced and quenched moments are virtually on top of each other as seen in the inset.

The additional effect of multiple scattering, *i.e.* due to interference between the two Fe monolayers, is seen from the difference between the superimposed curves and the full calculation of the total moments in Fig.(1). This difference corresponds to the magnetic moments calculated from the ΔG_{QW}^{σ} terms in eq.(2). In both situations the magnetic moment oscillates when the multiple scattering

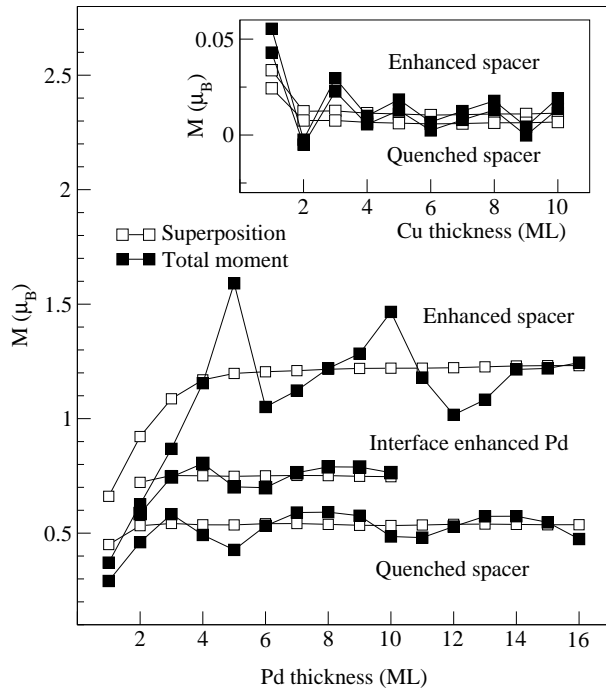


FIG. 1: The total magnetic moment of the spacer as calculated by a superposition of magnetic profiles and by doing a self consistent calculation of the system, both for quenched and enhanced Pd spacer layers. The difference between the curves calculated by a superposition indicates a giant magnetic enhancement (GME) effect of about $0.7 \mu_B$ arising from the non interacting Fe layers. By comparing total moments for the enhanced and quenched calculations the interference contribution to the GME can be estimated. The inset shows the same calculation for the Co/Cu system.

contribution is added with a period that is compatible with the Fermi surface nesting vector of Pd (5.7 ML) [1, 6]. By inspecting the three cases in Fig.(1) one can see that the enhancement introduces a phase shift of the magnetization oscillation. At the same time the enhancement changes the character of the curve to be more sawtooth shaped. Note that the sawtooth shape does not appear in the intermediate case, with interface enhanced Pd, where the band matching at the interfaces is very similar to the enhanced case.

Quantum well states

The big effect on the magnetization from multiple scattering is an indication of QW states in the spacer as was shown by Niklasson *et al* [14]. In order to investigate this possibility we have calculated the spectral density along the line $\bar{\Gamma} - \bar{M}$ in the 2 dimensional Brillouin zone for all different configurations and spacer thicknesses as illustrated in Fig.(2) for some cases. The QW states can be identified by the change in energy as function of spacer

thickness and we find very pronounced states in this system. The first thing we see by looking at all states for all spacer thicknesses is the counter intuitive effect that the aliasing moves the states up in energy with increasing spacer thickness. Secondly, the QW states in the spin-up channel has almost no dispersion at all whereas the spin-down state is divided into two disperse parts due to weak hybridization with Fe at the interfaces. We interpret this as an indication that the spin up state will influence the system to a greater extent than the spin down state.

For the AFM case, only the spectral density for the quenched calculation is shown. The reason is that we have not found any AFM case where the positions of the QW states differ between the enhanced and quenched calculations. The similarity is probably due to the fact that the total magnetic moment of the Pd spacer in the AFM system is always constrained to be zero by symmetry.

In the quenched calculations of the FM systems we always find spin split QW states that are shifted in the opposite direction to the bands *i.e.* the spin down state is shifted down in energy as compared to the spin up state. This can be explained by the different boundary conditions at the interfaces for the two spin channels.

In the enhanced FM systems the biggest effect on the QW state is the $0.7 \mu_B$ polarization that was found in Fig.(1) to be caused by the Fe layers when the interlayer interaction is neglected. The polarization is the same for all thicknesses above 5 ML resulting in a shift towards lower energies of the spin up QW states. When the states are shifted they will pass the Fermi energy at a larger spacer thickness compared to the quenched case, resulting in a phase shift as can be seen by comparing Fig.(2) and Fig.(1) for the 5 ML case. For this spacer thickness, the spin up state has not passed the Fermi energy in the enhanced case but is just above in the quenched case.

The sawtooth shape of the magnetization in Fig.(1) looks very similar to the change in integrated density of states between the continuous and quantized situations in the article by Bruno [8] Fig.(2). There the sawtooth shape is originating from large reflection coefficients at the interfaces. Coefficients close to one gives the sawtooth shape whereas smaller values result in a sinusoidal shape similar to our results for the completely quenched case. An equivalent way of explaining the two shapes in Brunos article is that with complete reflection the QW state in the spacer will contribute like a delta function to the DOS of the spacer. When the spacer thickness is changed, the entire QW state will pass the Fermi energy and give a step contribution to the integrated DOS which means a sawtooth shaped change in integrated DOS. If the reflection coefficients decrease, the delta function will be smeared out in energy. Hence, the step in integrated DOS will be smeared and the change in integrated DOS will be smoothed towards a sinusoidal shape.

In our case we do not expect the reflection coefficients to change when the enhancement is introduced. This

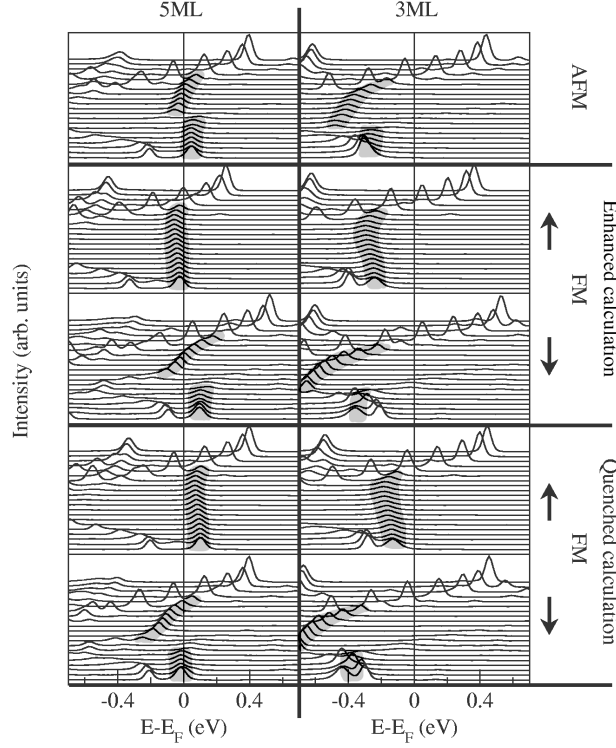


FIG. 2: The \bar{k} -resolved spectral density of a 5 ML and 3 ML system for the FM and AFM configuration. The lower block is the quenched and the middle block the enhanced calculation. Each part of the figure contains several curves where the lowest one is the spectral density at the $\bar{\Gamma}$ point. The other curves are also the spectral density but at \bar{k} -points shifted in the \bar{M} -direction. The curves are individually shifted in the y-direction in order to be plotted in the same graph. The QW states can be seen as distinct peaks with a small dispersion and have been shaded for clarity. The AFM result is very similar for the quenched and enhanced calculation and only the quenched result is shown here. The arrows indicate the different spin channels. The thin vertical lines indicate the Fermi energy in all graphs.

is confirmed both by the interface enhanced calculation in Fig.(1) where the shape of the magnetization curve is sinusoidal but the band matching at the Fe/Pd interface is very similar to the fully enhanced case, and also by the similar shapes of the QW states in Fig.(2). From these observations we conclude that the system uses the extra freedom to split the bands in order to avoid the smeared QW state at the Fermi energy. The result is effectively the same as if the reflection coefficients at the interfaces were close to unity.

MIC and enhancement

Because of the GME effect in the system arising from each Fe interface separately and the additional magnetization from the interface interference we may expect a very large effect on the magnetic interlayer coupling. The MIC of the $\text{Pd}_\infty/\text{Fe}_1/\text{Pd}_N/\text{Fe}_1/\text{Pd}_\infty$ system is shown in Fig.(3). The two curves are the results of the enhanced total energy calculation and the quenched calculation. Corresponding calculations for the

$\text{Cu}_\infty/\text{Co}_1/\text{Cu}_N/\text{Co}_1/\text{Cu}_\infty$ system is shown in the inset for comparison. The Co/Cu results are consistent with earlier calculations [29].

Both the two MIC results, with quenched Pd moments and enhanced moments show the same period between 5 and 6 ML as would be expected from RKKY theory in the limit of infinite spacer thickness. The largest difference between the two cases is that the quenched result oscillates around zero comparably to the Co/Cu system and does not show the FM bias that is present in the enhanced calculation. Also the decays with increasing spacer thickness are very different. By performing a fit to the decaying function $n^{-\alpha}(C \sin(\beta n + \Phi) + \xi)$ for values $n > 3$ we obtain $\alpha \approx 0.9$, $C \approx 45$, $\beta \approx 1.03$, $\Phi \approx 3.32$ and $\xi \approx 38$ for the enhanced case and $\alpha \approx 2.0$, $C \approx 136$, $\beta \approx 1.13$, $\Phi \approx 1.78$ and $\xi \approx -87$ for the quenched case. It is not clear if $n > 3$ is enough to reach outside the preasymptotic region and the values may have to be taken as qualitative asymptotic results. Nevertheless, there is a big difference in α which indicates that the coupling is of longer range in the enhanced case. There is also a phase shift analogous to the magnetization results. Additionally, the strength of the FM peaks at 4 ML and

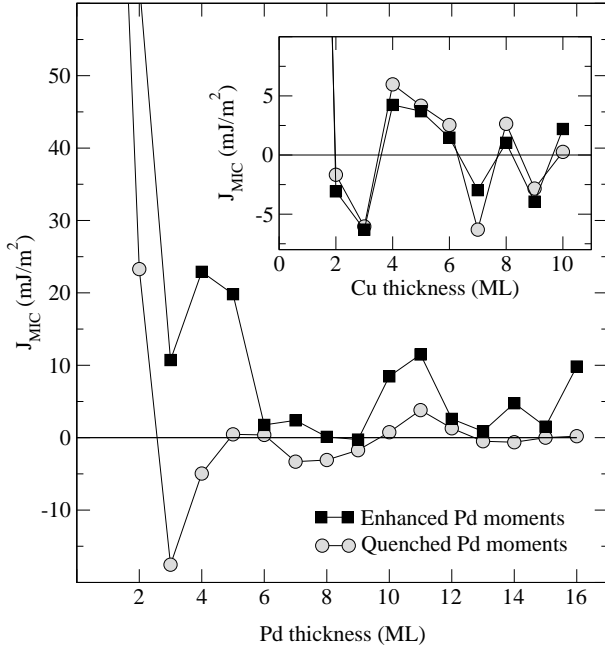


FIG. 3: The MIC of the $\text{Pd}_\infty/\text{Fe}_1/\text{Pd}_N/\text{Fe}_1/\text{Pd}_\infty$ system for the quenched and enhanced calculations. The inset shows the results for the corresponding Co/Cu system.

11 ML is strongly reduced in the quenched case. The differences must be attributed to the exchange enhancement in the Pd spacer which thus has large qualitative as well as quantitative effect on the MIC.

In order to determine for which configuration the enhancement has the largest effect we have calculated the difference in total energy between the enhanced (e) and the quenched (q) calculations for the AFM and FM systems separately. The formula $\Delta E_{A(F)}^{\text{tot}} = E_{A(F)}^e - E_{A(F)}^q$ was used where A and F denotes the antiferromagnetic and ferromagnetic configurations, respectively. The result is displayed in Fig.(4) and it is evident that the system always lowers its energy when the quenching is removed. The lowering of the energy is almost the same for all thicknesses above 4 ML in the AFM case but shows a similar oscillating structure as the enhanced MIC for the FM case. One can also see that the system always lowers its energy more in the FM configuration than in the AFM. From this observation we may draw the conclusion that the strong FM peaks of the MIC as well as the FM bias originates from the magnetic enhancement in the FM configured system. Note that it is very unlikely to be an effect of changed Fe magnetization, since we find almost the same moment for the Fe in the enhanced and quenched calculations (see Table I). We have also shown that the two cases has very similar reflection coefficients so this possibility is also excluded.

The energy gain by splitting the bands is of course larger if the Fe layers at the interfaces have high magnetic moments and thus induces high local moments on

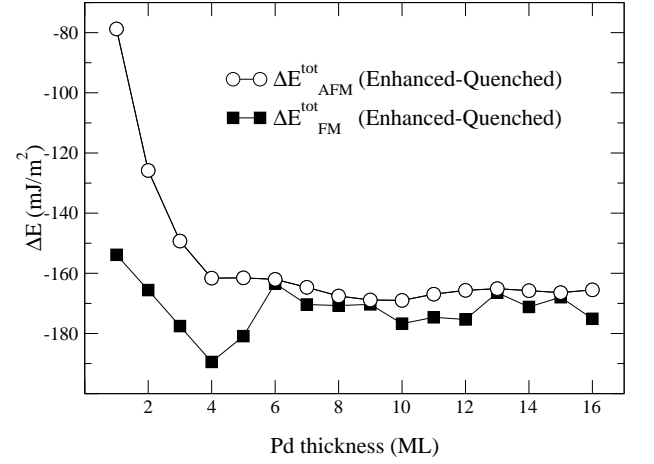


FIG. 4: The energy gain due to the exchange enhancement in the FM and AFM configurations. The only case that contributes to the strong positive peaks in the MIC is the FM configuration.

the Pd atoms. Then by reducing the magnetic moments at the Fe interfaces, for example by growing a few more fcc layers or by growing a thicker Fe film in the bcc structure, it may be possible to reduce the FM bias and thus obtain a weak AFM coupling in the region $6 \leq N \leq 9$. The MIC of the quenched case should be well described by conventional RKKY/QW models. However, the drastic difference between these calculations and the full calculation imply that the latter is not described by these models.

SUMMARY

We have investigated the magnetic properties of Fe/Pd fcc (100) systems and found a giant magnetic enhancement (GME) effect on the induced moments. We have estimated the effect of the GME on the MIC for Fe/Pd/Fe bilayer systems and concluded that the paramagnetic groundstate of the spacer is modified to such an extent that perturbation theories like RKKY and the QW model for the MIC may not be straightforward to apply. In particular, the overall FM bias, the asymptotic decay and the phase shift may not be captured. In the same bilayer system we have also found very strong QW induced magnetic enhancement on the same order of magnitude as the GME effect. We suggest that the strength of the magnetic moments at the interfaces in the Fe/Pd/Fe system may determine if an AFM coupling can be observed.

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